



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:02 AM GMT

PDB ID : 4A3K
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A
7NT DNA-RNA HYBRID
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

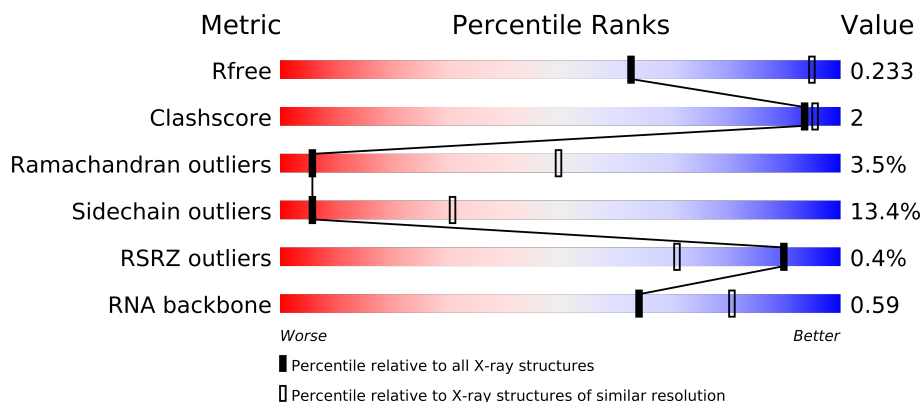
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1732	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	11	
14	P	7	
15	T	26	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31940 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

- Molecule 14 is a RNA chain called 5'-R(*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	7	Total	C	N	O	P	0	0	0
			152	68	31	46	7			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DTP*TP*TP*CP*CP*BRU*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			385	1	185	60	120	19		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

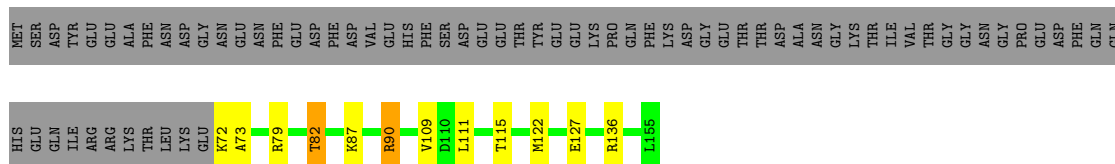
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

Chain E: 



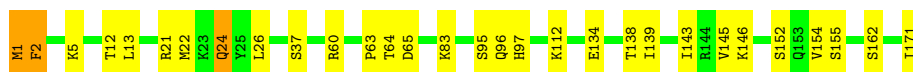
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 



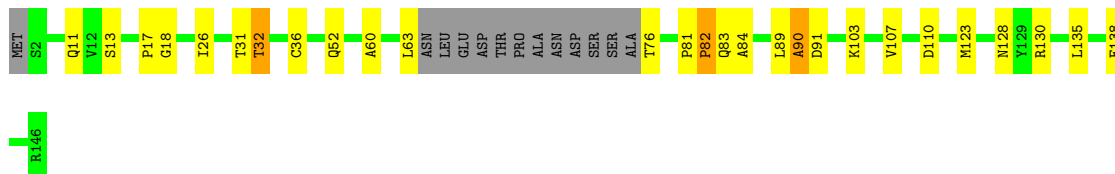
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 



- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 



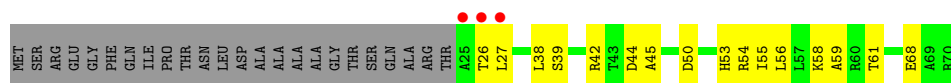
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 



- Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'

Chain N: 



- Molecule 14: 5'-R(*AP*CP*CP*AP*GP*GP*AP)-3'

Chain P: 

There are no outlier residues recorded for this chain.

- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DTP*TP*TP*CP*CP*BRU*GP*GP*TP*CP*AP*TP*T)-3'

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.91Å 391.36Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 3.50 49.11 – 3.37	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-3.50) 98.2 (49.11-3.37)	Depositor EDS
R_{merge}	1.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.158 , 0.185 0.221 , 0.233	Depositor DCC
R_{free} test set	3055 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.8	EDS
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 169418 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31940	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	1/11374 (0.0%)	0.84	8/15383 (0.1%)
2	B	0.51	0/9029	0.80	2/12171 (0.0%)
3	C	0.50	0/2133	0.80	2/2891 (0.1%)
4	D	0.52	0/1444	0.82	1/1935 (0.1%)
5	E	0.47	0/1788	0.72	0/2406
6	F	0.61	0/691	0.80	0/933
7	G	0.50	0/1368	0.83	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.46	0/989	0.80	0/1331
10	J	0.56	0/541	0.83	1/727 (0.1%)
11	K	0.48	0/938	0.73	0/1267
12	L	0.59	0/365	1.04	0/485
13	N	1.15	0/232	1.03	0/356
14	P	1.04	0/170	0.80	0/263
15	T	1.30	0/405	1.13	1/620 (0.2%)
All	All	0.55	1/32553 (0.0%)	0.82	15/44082 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	5.19	1.86	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	8.15	142.07	121.70
1	A	399	HIS	N-CA-CB	7.04	123.28	110.60
1	A	54	ASN	C-N-CA	6.02	136.75	121.70
1	A	35	ILE	N-CA-CB	5.82	124.19	110.80
1	A	56	PRO	C-N-CA	5.70	135.96	121.70
2	B	628	THR	C-N-CA	5.68	135.90	121.70
1	A	194	ALA	C-N-CA	5.67	135.88	121.70
1	A	53	LEU	N-CA-CB	5.45	121.31	110.40
2	B	338	GLY	C-N-CA	5.27	134.87	121.70
4	D	25	ALA	C-N-CA	5.25	134.81	121.70
1	A	35	ILE	CB-CA-C	5.24	122.09	111.60
15	T	24	DG	O4'-C4'-C3'	-5.20	102.42	104.50
3	C	39	ALA	N-CA-C	5.17	124.97	111.00
3	C	183	TRP	N-CA-C	-5.01	97.48	111.00
10	J	5	VAL	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	0	19	1
2	B	8859	0	0	17	0
3	C	2095	0	0	4	0
4	D	1434	0	0	1	0
5	E	1752	0	0	1	0
6	F	679	0	0	2	0
7	G	1340	0	0	3	1
8	H	1068	0	0	3	0
9	I	971	0	0	0	1
10	J	532	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	920	0	0	3	0
12	L	363	0	0	0	0
13	N	207	0	0	1	0
14	P	152	0	0	0	0
15	T	385	0	0	1	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31940	0	0	50	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.86	1.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.30	0.65
1:A:53:LEU:CD2	1:A:54:ASN:N	2.63	0.62
2:B:996:ARG:NH2	3:C:174:ALA:O	2.32	0.62
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.33	0.61
7:G:1:MET:CE	7:G:2:PHE:N	2.67	0.57
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.54
2:B:296:GLU:O	2:B:300:HIS:CD2	2.61	0.54
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.41	0.54
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.53
2:B:882:THR:OG1	2:B:935:ARG:N	2.41	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.52
8:H:82:PRO:O	8:H:84:ALA:N	2.45	0.49
1:A:448:PRO:O	1:A:449:SER:CB	2.60	0.49
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.45	0.49
10:J:9:SER:OG	10:J:48:ARG:NH2	2.45	0.49
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.46	0.49
1:A:626:ASN:O	1:A:631:HIS:ND1	2.48	0.46
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.49	0.46
2:B:801:LYS:O	10:J:52:THR:OG1	2.35	0.45
1:A:385:ILE:O	1:A:389:THR:OG1	2.34	0.45
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.50	0.44
2:B:824:ILE:O	2:B:1009:ASP:N	2.50	0.44
10:J:48:ARG:O	10:J:52:THR:CG2	2.66	0.44
2:B:1167:GLY:O	2:B:1216:LEU:N	2.50	0.44
7:G:21:ARG:NH1	7:G:24:GLN:OE1	2.51	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.51	0.44
2:B:815:ARG:NH1	2:B:815:ARG:CG	2.81	0.44
3:C:75:MET:O	3:C:246:ARG:NH2	2.50	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.37	0.42
6:F:82:THR:O	6:F:136:ARG:NH1	2.53	0.42
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.53	0.42
13:N:4:DG:N2	15:T:15:DT:O2	2.53	0.42
4:D:10:THR:O	4:D:12:ARG:NH2	2.53	0.42
1:A:53:LEU:O	1:A:54:ASN:C	2.59	0.41
1:A:55:ASP:CG	1:A:55:ASP:O	2.59	0.41
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.79	0.41
8:H:82:PRO:C	8:H:84:ALA:N	2.74	0.41
1:A:469:ARG:NH2	2:B:991:GLY:O	2.54	0.41
6:F:90:ARG:NH1	6:F:90:ARG:CG	2.84	0.41
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.08	0.41
8:H:63:LEU:CB	8:H:90:ALA:CB	2.99	0.40
2:B:100:PRO:O	2:B:180:TYR:OH	2.39	0.40
1:A:868:TYR:CZ	1:A:1064:VAL:CG1	3.04	0.40
1:A:869:GLY:O	5:E:204:THR:CG2	2.69	0.40
1:A:399:HIS:O	1:A:401:GLY:N	2.54	0.40
1:A:64:ASN:O	1:A:65:LEU:CB	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:904:THR:N	9:I:33:SER:O[8_555]	2.18	0.02
7:G:95:SER:OG	7:G:97:HIS:CD2[3_654]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1732 (82%)	1252 (88%)	112 (8%)	50 (4%)	6	50
2	B	1095/1224 (90%)	969 (88%)	82 (8%)	44 (4%)	5	44
3	C	264/318 (83%)	236 (89%)	24 (9%)	4 (2%)	15	69
4	D	174/221 (79%)	154 (88%)	14 (8%)	6 (3%)	6	50
5	E	212/215 (99%)	186 (88%)	24 (11%)	2 (1%)	25	80
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	19	75
7	G	169/171 (99%)	160 (95%)	6 (4%)	3 (2%)	13	65
8	H	129/146 (88%)	101 (78%)	19 (15%)	9 (7%)	2	26
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	8	57
10	J	63/70 (90%)	55 (87%)	4 (6%)	4 (6%)	2	29
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	3
All	All	3876/4564 (85%)	3421 (88%)	321 (8%)	134 (4%)	6	50

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	399	HIS
1	A	448	PRO
1	A	449	SER
1	A	1175	SER
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	473	MET

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Mol	Chain	Res	Type
2	B	629	ASP
2	B	707	PRO
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	1066	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	215	GLU
3	C	240	VAL
4	D	18	VAL
9	I	9	ASP
10	J	6	ARG
12	L	53	HIS
12	L	56	LEU
1	A	54	ASN
1	A	76	GLU
1	A	178	GLY
1	A	187	LYS
1	A	189	ARG
1	A	195	ASP
1	A	311	GLN
1	A	312	PRO
1	A	1124	HIS
1	A	1206	ASP
1	A	1281	ARG
2	B	340	ALA
2	B	341	LEU
2	B	466	TRP
2	B	867	GLY
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
2	B	1190	ASP
4	D	169	SER
8	H	17	PRO
8	H	81	PRO
8	H	83	GLN
9	I	95	THR
10	J	2	ILE
10	J	55	ASP
12	L	39	SER

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Mol	Chain	Res	Type
12	L	50	ASP
1	A	43	GLU
1	A	167	CYS
1	A	251	SER
1	A	336	ILE
1	A	593	GLU
1	A	1173	HIS
1	A	1255	GLU
2	B	343	ILE
2	B	575	PRO
2	B	883	LEU
2	B	1223	ASP
4	D	16	LYS
4	D	52	LEU
4	D	199	ASN
5	E	3	GLN
7	G	154	VAL
8	H	52	GLN
8	H	60	ALA
8	H	82	PRO
10	J	17	LYS
12	L	45	ALA
1	A	35	ILE
1	A	62	ASP
1	A	283	GLY
1	A	331	GLY
1	A	423	ASP
1	A	567	LYS
1	A	569	LYS
1	A	775	ILE
1	A	1122	PRO
2	B	262	GLU
2	B	338	GLY
2	B	449	ASN
2	B	533	CYS
2	B	711	GLU
3	C	150	GLY
4	D	220	LEU
7	G	63	PRO
8	H	18	GLY
8	H	90	ALA
9	I	105	SER

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Mol	Chain	Res	Type
12	L	38	LEU
12	L	59	ALA
1	A	52	GLY
1	A	156	ASP
1	A	958	VAL
1	A	1437	GLY
2	B	368	GLU
2	B	772	ALA
2	B	792	MET
2	B	1155	SER
6	F	73	ALA
7	G	139	ILE
8	H	32	THR
12	L	26	THR
2	B	1108	ARG
3	C	38	ILE
2	B	108	VAL
5	E	90	VAL
1	A	196	GLU
2	B	168	GLY
2	B	251	ILE
2	B	436	VAL
2	B	902	GLY
2	B	907	GLY
2	B	369	GLY
1	A	1123	GLY
2	B	1214	PRO
1	A	55	ASP
2	B	231	PRO
2	B	364	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1519 (82%)	1070 (86%)	170 (14%)	5	29
2	B	966/1061 (91%)	845 (88%)	121 (12%)	7	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	234/274 (85%)	207 (88%)	27 (12%)	8	39
4	D	160/200 (80%)	131 (82%)	29 (18%)	2	15
5	E	196/197 (100%)	176 (90%)	20 (10%)	11	48
6	F	74/137 (54%)	64 (86%)	10 (14%)	6	30
7	G	152/152 (100%)	128 (84%)	24 (16%)	4	23
8	H	117/128 (91%)	100 (86%)	17 (14%)	5	27
9	I	113/116 (97%)	100 (88%)	13 (12%)	8	39
10	J	60/65 (92%)	51 (85%)	9 (15%)	4	26
11	K	99/102 (97%)	85 (86%)	14 (14%)	5	28
12	L	40/57 (70%)	32 (80%)	8 (20%)	2	11
All	All	3451/4008 (86%)	2989 (87%)	462 (13%)	6	31

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	44	THR
1	A	47	ARG
1	A	50	ILE
1	A	62	ASP
1	A	64	ASN
1	A	65	LEU
1	A	67	CYS
1	A	84	ILE
1	A	88	LYS
1	A	93	VAL
1	A	96	ILE
1	A	117	GLU
1	A	126	LEU
1	A	132	LYS
1	A	141	LEU
1	A	144	THR
1	A	157	ASP

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	174	ILE
1	A	185	TRP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	226	GLU
1	A	252	PHE
1	A	261	ASP
1	A	265	LYS
1	A	270	LEU
1	A	307	ASP
1	A	315	LEU
1	A	324	SER
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	408	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU

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Mol	Chain	Res	Type
1	A	500	GLU
1	A	518	LYS
1	A	527	THR
1	A	532	ARG
1	A	538	ASP
1	A	541	ILE
1	A	544	ASP
1	A	549	MET
1	A	555	ASP
1	A	566	ILE
1	A	569	LYS
1	A	571	LEU
1	A	577	ILE
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	644	LYS
1	A	666	ILE
1	A	672	ASP
1	A	675	THR
1	A	685	GLU
1	A	702	LEU
1	A	738	LYS
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	821	ARG
1	A	824	LEU
1	A	826	ASP
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	885	THR
1	A	886	ILE

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Mol	Chain	Res	Type
1	A	904	THR
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	941	LYS
1	A	948	VAL
1	A	973	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1015	VAL
1	A	1024	SER
1	A	1029	ARG
1	A	1036	ARG
1	A	1064	VAL
1	A	1067	LEU
1	A	1116	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1128	GLN
1	A	1135	ARG
1	A	1145	SER
1	A	1173	HIS
1	A	1176	LEU
1	A	1192	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1256	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1266	THR
1	A	1277	GLU
1	A	1293	SER
1	A	1295	THR

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Mol	Chain	Res	Type
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1376	THR
1	A	1383	SER
1	A	1386	ARG
1	A	1391	ARG
1	A	1400	CYS
1	A	1405	THR
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1454	MET
2	B	21	GLU
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	102	VAL
2	B	109	THR
2	B	118	ARG
2	B	134	LYS
2	B	178	ASN
2	B	185	THR
2	B	187	SER
2	B	217	ARG
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	280	ILE
2	B	289	LEU
2	B	294	ASP
2	B	298	LEU
2	B	313	MET

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Mol	Chain	Res	Type
2	B	323	VAL
2	B	336	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	350	GLN
2	B	351	TYR
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	436	VAL
2	B	446	LEU
2	B	452	THR
2	B	453	ILE
2	B	469	GLN
2	B	470	LYS
2	B	476	ARG
2	B	481	GLN
2	B	485	ARG
2	B	486	TYR
2	B	537	LYS
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	606	LYS
2	B	616	ILE
2	B	620	ARG

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Mol	Chain	Res	Type
2	B	624	LEU
2	B	628	THR
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	682	SER
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	797	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	884	ARG
2	B	889	THR
2	B	904	ARG
2	B	908	GLU
2	B	933	SER
2	B	934	LYS
2	B	964	VAL
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1050	ILE
2	B	1060	ARG

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Mol	Chain	Res	Type
2	B	1062	HIS
2	B	1065	GLN
2	B	1072	MET
2	B	1106	ARG
2	B	1128	LEU
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1156	ASP
2	B	1160	VAL
2	B	1175	LEU
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1202	LEU
3	C	3	GLU
3	C	16	ASP
3	C	25	VAL
3	C	26	ASP
3	C	50	GLU
3	C	52	GLU
3	C	55	THR
3	C	66	ARG
3	C	81	GLU
3	C	89	GLU
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	148	ARG
3	C	155	LEU
3	C	163	ILE
3	C	215	GLU
3	C	237	SER
3	C	240	VAL
3	C	259	LEU

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Mol	Chain	Res	Type
3	C	265	MET
4	D	5	THR
4	D	7	THR
4	D	10	THR
4	D	12	ARG
4	D	17	LYS
4	D	18	VAL
4	D	22	GLU
4	D	23	ASN
4	D	27	LEU
4	D	32	GLU
4	D	35	LEU
4	D	41	GLN
4	D	67	ARG
4	D	118	THR
4	D	123	LEU
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	159	THR
4	D	166	LEU
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	213	GLU
4	D	219	THR
5	E	31	THR
5	E	41	ASP
5	E	49	SER
5	E	57	MET
5	E	67	GLU
5	E	69	ILE
5	E	84	ASP
5	E	92	THR
5	E	99	HIS
5	E	104	ASN
5	E	113	GLN
5	E	146	HIS

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Mol	Chain	Res	Type
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	190	LEU
5	E	192	ARG
5	E	196	VAL
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
6	F	122	MET
6	F	127	GLU
7	G	1	MET
7	G	2	PHE
7	G	5	LYS
7	G	12	THR
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	37	SER
7	G	60	ARG
7	G	64	THR
7	G	65	ASP
7	G	83	LYS
7	G	96	GLN
7	G	112	LYS
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	146	LYS
7	G	152	SER
7	G	155	SER
7	G	162	SER
7	G	171	ILE

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Mol	Chain	Res	Type
8	H	11	GLN
8	H	13	SER
8	H	26	ILE
8	H	31	THR
8	H	32	THR
8	H	36	CYS
8	H	76	THR
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	107	VAL
8	H	110	ASP
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	7	CYS
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	42	LEU
9	I	43	VAL
9	I	50	THR
9	I	74	GLU
9	I	83	ASN
9	I	91	ARG
9	I	92	ARG
9	I	106	CYS
9	I	120	GLN
10	J	2	ILE
10	J	6	ARG
10	J	12	LYS
10	J	13	VAL
10	J	22	LEU
10	J	23	ASN
10	J	34	THR
10	J	42	LYS
10	J	48	ARG
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS

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Mol	Chain	Res	Type
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	34	THR
11	K	37	LYS
11	K	47	ARG
11	K	51	LEU
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	113	THR
12	L	27	LEU
12	L	42	ARG
12	L	44	ASP
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	6/7 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	15,14	19,21,22	1.22	3 (15%)	22,30,33	2.66	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15,14	-	0/5/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C6-N1	2.59	1.40	1.34
15	T	22	BRU	C2-N3	-2.18	1.33	1.37
15	T	22	BRU	P-OP1	2.06	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C6-N1-C2	-10.02	119.56	122.41
15	T	22	BRU	O4'-C1'-N1	5.43	117.89	107.68
15	T	22	BRU	C2'-C1'-N1	-3.57	104.82	114.08
15	T	22	BRU	N3-C2-N1	2.89	118.39	115.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1422/1732 (82%)	0.05	6 (0%) 90 71	52, 99, 156, 225	0
2	B	1115/1224 (91%)	0.08	3 (0%) 91 76	59, 109, 169, 210	0
3	C	266/318 (83%)	-0.01	0 100 100	71, 97, 136, 170	0
4	D	178/221 (80%)	0.20	1 (0%) 86 59	75, 111, 171, 186	0
5	E	214/215 (99%)	0.13	1 (0%) 88 64	75, 132, 177, 194	0
6	F	84/155 (54%)	-0.05	0 100 100	58, 79, 110, 126	0
7	G	171/171 (100%)	0.13	0 100 100	67, 98, 134, 153	0
8	H	133/146 (91%)	0.37	0 100 100	109, 140, 177, 200	0
9	I	119/122 (97%)	0.10	2 (1%) 67 34	105, 136, 174, 191	0
10	J	65/70 (92%)	-0.04	0 100 100	79, 94, 139, 159	0
11	K	115/120 (95%)	0.06	1 (0%) 81 51	69, 96, 132, 148	0
12	L	46/70 (65%)	0.70	3 (6%) 18 8	85, 165, 184, 194	0
13	N	10/11 (90%)	0.21	0 100 100	173, 193, 239, 248	0
14	P	7/7 (100%)	-0.25	0 100 100	101, 108, 155, 173	0
15	T	19/26 (73%)	0.16	0 100 100	125, 159, 250, 251	0
All	All	3964/4608 (86%)	0.09	17 (0%) 90 71	52, 105, 169, 251	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	5.9
12	L	25	ALA	4.6
2	B	883	LEU	4.2
1	A	257	ARG	3.6
1	A	1455	PRO	3.6
12	L	26	THR	3.6
1	A	1176	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	340	ALA	3.3
1	A	194	ALA	3.1
4	D	13	ARG	3.1
1	A	256	GLN	2.6
9	I	118	ARG	2.6
11	K	115	ALA	2.3
2	B	167	ILE	2.2
9	I	119	THR	2.2
5	E	123	LEU	2.0
1	A	161	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.12	-1.64	123,129,133,134	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
16	ZN	I	1121	1/1	0.13	-0.15	125,125,125,125	0
16	ZN	A	2457	1/1	0.16	-0.95	72,72,72,72	0
16	ZN	B	2225	1/1	0.17	-1.06	82,82,82,82	0
16	ZN	I	1122	1/1	0.05	-1.46	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	C	1269	1/1	0.09	-1.65	84,84,84,84	0
16	ZN	A	2456	1/1	0.07	-1.82	127,127,127,127	0
16	ZN	J	1066	1/1	0.20	-1.91	82,82,82,82	0
16	ZN	L	1071	1/1	0.06	-3.23	192,192,192,192	0
17	MG	A	2458	1/1	0.12	-3.57	78,78,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.